Random-phase approximation plus second-order screened exchange applied to extended systems

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The use of wave function based methods, such as coupled-cluster theory [1], to add electronic correlation to the Hartree-Fock (HF) approximation is common practice in the computational quantum chemistry of molecular systems. Due to the computational cost involved, however, these methods have hardly been applied to extended systems.

We have implemented an approximation to the coupled-cluster doubles (CCD) theory including only ring diagrams in the amplitude equations within the framework of the full-potential Projector-Augmented-Wave (PAW) method [2], using periodic boundary conditions and a plane wave basis set. The method goes beyond the so-called direct-random-phase approximation (RPA) [see Fig. 1(a)], since it incorporates an exchange-like term that originates from the CCD energy expression [3]. The latter we term second-order screened exchange [SOSEX, see Fig. 1(b)]. We show that the inclusion of SOSEX to the direct-random-phase approximation allows for a very accurate description of electronic correlation in atoms and solids.

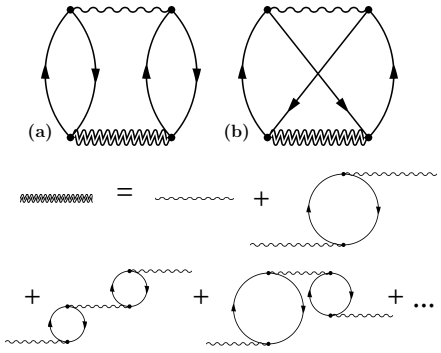

Figure 1: Diagrams corresponding to (a) direct-RPA correlation and (b) second-order screened exchange (SOSEX). The wiggly and double wiggly line represent the unscreened and screened Coulomb interaction, respectively.

[1] J. Čížek, J. Phys. Chem. **45**, 4256 (1966).
[2] P. E. Blöchl, "Projector augmented-wave method," Phys. Rev. B **50**, 17953 (1994).
[3] D. L. Freeman, Phys. Rev. B **15**, 5512 (1977).